WHAT IS CLAIMED IS:

1   1.   A method for pharmacological computational model construction, comprising:

2   (a)   presenting a graphical user interface having a plurality of objects, each

3   object representing one or both of a pharmacokinetic element and a

4   pharmacodynamic element;

5   (b)   receiving instructions via the graphical user interface for connection of at

6   least two of the objects;

7   (c)   displaying the at least two objects connected in accordance with the

8   received instructions;

9   (d)   converting the at least two connected objects into equations corresponding

10   to the pharmacokinetic and pharmacodynamic elements represented by the

11   at least two connected objects, wherein the converting step (d) occurs

12   substantially coincident with the object displaying step (c); and

13   (e)   displaying the equations on the graphical user interface substantially

14   coincident with the object displaying step (c).

1   2.   The method of claim 1, wherein the converting step (d) comprises:

2   (f)   converting the at least two connected objects into an internal format; and

3   (g)   converting the internal format into a surface syntax.

1   3.   The method of claim 2, wherein the surface syntax represents differential

2   equations in an integrator equals rate expression format.

1   4.   The method of claim 2, wherein the objects comprise one of more of

2   compartment blocks, flow blocks, response blocks, and formulation blocks.

1   5.   A method for pharmacological computational model construction, comprising:

2   (a)   presenting a graphical user interface having a plurality of objects, each

3   object representing one or both of a pharmacokinetic element and a

4   pharmacodynamic element;

5   (b)   receiving instructions via the graphical user interface for connection of at

6   least two of the objects;

7   (c)   displaying the at least two objects connected in accordance with the

8   received instructions;

9   (d)   converting the at least two connected objects into an internal format

10   corresponding to the pharmacokinetic and pharmacodynamic elements

11   represented by the at least two connected objects, wherein the converting

12   step (d) occurs substantially coincident with the object displaying step (c);

13   (e)   interpreting the internal format to generate a time-based simulation

14   including calculation of one or more selected variables;

15   (f)   plotting the one or more selected variables in a graph; and

16   (g)   repeating the interpreting and plotting steps (e) and (f), thereby actively

17   updating the graph as the instructions are received in step (b).

1   6.   The method of claim 5, further comprising:

2   (h)   receiving commands via the graphical user interface to modify at least one

3   of the one or more selected variables; and

4   (i)   modifying the interpreting step (e) in response to the received commands

5   in step (b); thereby actively updating the graph to reflect changes to the at

6   least one of the one or more selected variables.

1   7.   The method of claim 6, wherein the modifying step (i) comprises revising the

2   internal format.

1   8.   The method of claim 6, wherein one or more of the one or more selected

2   variables depend upon a random variable, wherein the interpreting step (e) generates a

3   value for the random variable upon each repetition, and wherein the plotting step (f) plots

4   the one or more selected variables over plots from previous repetitions, thereby showing

5   variability of the one or more selected variables caused by the random variable within a

6   single graph.

1   9.   The method of claim 6, wherein the internal format comprises a parse tree.

1 10. The method of claim 6, wherein the one or more selected variables comprise

2 at least two selected variables, and wherein the plotting step (f) comprises plotting at least

3 one selected variable versus another selected variable.

1 11. The method of claim 6, wherein the plotting step (f) comprises plotting the

2 one or more selected variables versus time.

1 12. The method of claim 5, further comprising:

2 (j) translating the internal format into text strings representing equations, the

3   equations corresponding to the respective pharmacokinetic and

4   pharmacodynamic elements represented by the two or more connected

5   objects; and

6 (k) displaying the text strings substantially coincident with the object

7   displaying step (c).

1 13. The method of claim 12, wherein the objects comprise one or more of

2 compartment blocks, flow blocks, response blocks, and formulation blocks.

1 14. A computer readable medium having stored thereon one or more sequences of

2 instructions for causing one or more processors to perform steps for enabling construction

3 of a graphical pharmacological computational model, the steps comprising:

4 (a) presenting a graphical user interface having a plurality of objects, each

5   object representing one or both of a pharmacokinetic element and a

6   pharmacodynamic element;

7 (b) receiving instructions via the graphical user interface for connection of at

8   least two of the objects;

9 (c) displaying the at least two objects connected in accordance with the

10   received instructions;

11 (d) converting the at least two connected objects into equations corresponding

12   to the pharmacokinetic and pharmacodynamic elements represented by the

13   at least two connected objects, wherein the converting step (d) occurs

14   substantially coincident with the object displaying step (c); and

15   (e)   displaying the equations on the graphical user interface substantially

16   coincident with the object displaying step (c).

1   15. The computer readable medium of claim 14, wherein the converting step (d)

2 comprises:

3   (f)   converting the at least two connected objects into an internal format; and

4   (g)   converting the internal formal into a surface syntax.

1   16. A computer readable medium having stored thereon one or more sequences of

2 instructions for causing one or more processors to perform steps for enabling construction

3 of a graphical pharmacological computational model, the steps comprising:

4   (a)   presenting a graphical user interface having a plurality of objects, each

5   object representing one or both of a pharmacokinetic element and a

6   pharmacodynamic element;

7   (b)   receiving instructions via the graphical user interface for connection of at

8   least two of the objects;

9   (c)   displaying the at least two objects connected in accordance with the

10   received instructions;

11   (d)   converting the at least two connected objects into an internal format

12   corresponding to the pharmacokinetic and pharmacodynamic elements

13   represented by the at least two connected objects, wherein the converting

14   step (d) occurs substantially coincident with the object displaying step (c);

15   (e)   interpreting the internal format to generate a time-based simulation

16   including calculation of one or more selected variables;

17   (f)   plotting the one or more selected variables in a graph; and

18   (g)   repeating the interpreting and plotting steps (e) and (f), thereby actively

19   updating the graph as the instructions are received in step (b).

1   17. The computer readable medium of claim 16, wherein the steps further

2 comprise:

3   (h)   receiving commands via the graphical user interface to modify at least one

4   of the one or more selected variables; and

5   (i)   modifying the interpreting step (e) in response to the received commands

6   in step (b; thereby actively updating the graph to reflect changes to the at

7   least one of the one or more selected variables.

1   18. The computer readable medium of claim 17, wherein one or more of the one

2 or more selected variables depend upon a random variable, wherein the interpreting step

3 (e) generates a value for the random variable upon each repetition, and wherein the

4 plotting step (f) plots the one or more selected variables over plots from previous

5 repetitions, thereby showing variability of the one or more selected variables caused by

6 the random variable within a single graph.

1   19. The computer readable medium of claim 17, wherein the plotting step (f)

2 comprises plotting the one or more selected variables versus time.

1   20. The computer readable medium of claim 16, wherein the steps further

2 comprise:

3   (j)   translating the internal format into text strings representing equations, the

4   equations corresponding to the respective pharmacokinetic and

5   pharmacodynamic elements represented by the two or more connected

6   objects; and

7   (k)   displaying the text strings substantially coincident with the object

8   displaying step (c).

1   21. A system configured to present a graphical user interface having a plurality of

2 objects, each object representing one or both of a pharmacokinetic element and a

3 pharmacodynamic element, the graphical user interface enabling construction of a

4 graphical pharmacological computational model, the system comprising:

5   (a)   a processor;

6   (b)   a data storage area; and

7   (c)   an execution area configured to:

8	(i)	receive instructions regarding connection of at least two of the
9		objects;
10	(ii)	display the connected objects in accordance with the instructions;
11	(iii)	convert the at least two connected objects into an internal format
12		corresponding to the pharmacokinetic and pharmacodynamic
13		elements represented by the at least two connected objects, in
14		parallel with the object display;
15	(iv)	interpret the internal format to generate a time-based simulation
16		including calculation of one or more selected variables;
17	(v)	plot the one or more selected variables in a graph; and
18	(vi)	repeat the interpreting and plotting, thereby actively updating the
19		graph as the instructions are received.

1   22. The computer system of claim 21, wherein the execution area is further

2 configured to:

3	(a)	receive commands via the graphical user interface to modify at least one of
4		the one or more selected variables; and
5	(b)	modify the interpreting in response to the received commands; thereby
6		actively updating the graph to reflect changes to the at least one of the one
7		or more selected variables.

1   23. The computer system of claim 22, wherein one or more of the one or more

2 selected variables depend upon a random variable, and wherein the plots occur over

3 previous plots, thereby showing variability of the one or more selected variables caused

4 by the random variable within a single graph.

1   24. The computer system of claim 23, wherein the plots are of the one or more

2 selected variables versus time.

1   25. The computer system of claim 24, wherein each of the one or more selected

2 variables is plotted using a different color.

1   26. The computer system of claim 21, wherein the execution area is further

2 configured to:

3   (a)   translate the internal format into text strings representing equations

4   corresponding to the pharmacokinetic and pharmacodynamic elements

5   represented by the connected objects; and

6   (b)   display the text strings in parallel with the object display.